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Interfacial Atomic Arrangements in AlAs/GaAs Ultra-short-period Superlattices: An X-ray Scattering Study

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Beamline(s): X14A

Introduction: For large-period superlattices or multilayers, an interface is conventionally described by an interfacial layer of certain width, which could be caused by either physical "roughness" or chemical "intermixing" or both. Methods, such as x-ray reflection and diffuse scattering, have been developed to characterize the properties of the interfaces. If the interfaces are physically rough, they can be described by a r.m.s roughness and an in-plane correlation length; while if the interfaces experience chemical intermixing, they can be described by an interfacial composition profile characteristic of inter-diffusion or atom segregation. Both of these two features can be quantified by x-ray experiments. However, these descriptions cannot be applied to very thin layers of only several atomic monolayers (ML) thick because almost every atom can now be considered as at the interfaces. Thus, the interfaces of ultra-thin layers need to be described by more detailed interfacial atomic arrangements.

Methods and Materials: In this work, we used high-resolution X14A beamline to study the interfaces of a series of AlAs/GaAs ultra-short-period superlattices. These samples were grown by MBE on GaAs (001) substrates. The individual layer thickness ranges from 1 to 10 MLs. For convenience, a structure with *m* ML of AlAs and *n* ML of GaAs will be denoted by *m/n*. We used coplanar x-ray diffraction and measured the 2D intensity distribution around the superlattice reflections. To analyze the experimental data, a modified kinematic x-ray scattering theory is applied, which considers a 2D structure factor of an individual lattice planes with lateral domains of different composition due possibly to the non-planar growth of AlAs (Volmer-Weber growth).

Results: A 1/1 superlattice forms an artificial CuAu-I structure. Therefore, we may expect superlattices peaks at (00l) (l=1,3,5, …) in shape of a spot. However, the experimental data shows no (003) peak but two split peaks at ($003\pm\delta$). Moreover, these two peaks are spread along the HK or [110] in-plane direction. A 2/2 superlattice, in contrast, does show a single superlattice peak, but shifted away from the expected (002.5) position to (002.49). Again, the peak is broadened along the [110] direction. Results from a 4/4 and a 10/10 superlattice also differ from our expectation. To understand these results, theoretical modeling was made which considers both a periodic compositional faults in the growth direction, caused by a 5% error on growth rate, and an in-plane domain structures of an average size of 10-100 unit cells. From the fitting, we found that the interfaces of these ultra-short-period superlattices contain two features of very different length scale – one in atomic scale due to the Ga segregation and the other in nano-scale caused by non-planar growth of AlAs. More importantly, the interfaces in the AlAs/GaAs superlattices are asymmetric in both length scales. The direct interfaces (AlAs/GaAs) are smoother in nano-scale but rougher in atomic scale than the inverse interfaces (GaAs/AlAs).

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